

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

REMARKS

By the present Amendment, claims 5-12, 15, 16, and 19-21 have been amended, and claims 17-18 canceled. No claims have been added. Accordingly claims 5-16 and 19-21 remain pending in the application. Claims 5, 9, 10, 12, 20, and 21 are independent.

In the Office Action of October 23, 2003, claims 11, 13, 14, and 16-18 were rejected under 35 U.S.C. §112, first paragraph as failing to comply with the written description requirement. Claims 5-20 were rejected under 35 U.S.C. §101 as being directed to non-statutory subject matter. Claims 5-21 were rejected under 35 U.S.C. §112, second paragraph as being indefinite for failing to particularly point out and distinctly claim the subject matter regarded as the invention. Claims 5, 11, 15, and 20 were rejected under 35 U.S.C. §102(b) as being anticipated by Graovac et al. [JACS 95(19):6267-6273 (1973)]. Claims 5, 7, 8, 10, 11, 15, and 19-21 were rejected under 35 U.S.C. §102(b) as being anticipated by Morikawa [Computers Chem. 20:159-165 (1996)]. These rejections are respectfully traversed.

Claims 11, 13, 14, and 16-18 were rejected under 35 U.S.C. §112, first paragraph as failing to comply with the written description requirement. Specifically, the Office Action alleges that these claims contain subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the art that the inventors had possession of the claimed invention at the time the application was filed. The Office Action alleges that the limitation of "queuing at least a subset of candidates by priority" is not supported by the specification. The Office Action further indicates that the specification only supports priority queuing of ESVDs.

By the present Amendment, claim 11 has been amended to recite "queuing at least a subset of the ESVDs by priority." As indicated in the Office Action, the disclosure supports such a recitation. It is therefore respectfully submitted that, as amended, claim 11 satisfies the requirements of 35 U.S.C. §112, first paragraph.

The Office Action Alleges that claims 13 and 14 provide a table that is "configured to allow additional elements, etc. to be added", and that such a configuration is not found in the

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

application as filed. The Office Action further states that the disclosure does not show a table which is specifically configured to allow additional elements.

Applicant respectfully disagrees with the Examiner's conclusions regarding claims 13 and 14. First, the claims of the application should be viewed in light of the understandings of one skilled in the art. A skilled artisan would not interpret the table recited in claims 13 and 14 (and described in the disclosure) as limited to the exact size shown in the figure. It is well known and accepted that tables used to store information are dynamically configurable to accommodate the addition and removal of information. Applicant further directs attention to Figure 7 which explicitly specifies that the illustrated table shows selected electronic state/valence distributions. Additionally, the corresponding description indicates that the table "is not a complete list,..." See page 7, lines 5-6. Accordingly, a skilled artisan would readily recognize and appreciate that additional elements and values could be added. Further, the disclosure is intended to be illustrative, and not limiting. There is nothing in the disclosure to indicate that additional elements cannot be added to the table.

Applicant therefore respectfully submit that independent claims 13 and 14 are in full compliance with the requirements of 35 U.S.C. §112, first paragraph.

The Office Action indicates that claim 16 contains the limitation of "determining whether it is practical to produce a fixed bond representation of the structure," and that such a practical determination was not included in the disclosure as filed. The Office Action indicates that the disclosure only supports termination by exhaustion or exceeding an allocated amount of time. Claims 17 and 18 were rejected for having similar language.

By the present Amendment, claim 16 has been amended to specifically recite a step of "determining whether it is possible to produce a neutral, non-radical, fixed-bond representation of most chemical structures." Claim 16 now includes a practical limit that is not broad and generic, as suggested in the Office Action. Claims 17 and 18 have been deleted, thereby rendering this particular ground of rejection moot.

Applicant therefore respectfully requests withdrawal of this rejection.

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

Claims 5-20 were rejected under 35 U.S.C. §101 as being directed to non-statutory subject matter. In support of this rejection, the Office Action alleges that the present claims merely "manipulate chemical structure information and/or representation(s) without any physical transformation outside the computer.

Applicant respectfully disagree with this assertion. First, it does not appear that a *prima facie* case has been made. The M.P.E.P. specifically states that Office personnel have the burden of establishing that the claimed invention, as a whole, is directed solely to the manipulation of abstract ideas with no useful results. Furthermore, Office personnel are required to expressly show how the language of the claims has been interpreted to support the rejection. See M.P.E.P. §2106(II)(A). This case has not been made by the Office Action. Rather, only conclusory statements regarding the lack of usefulness has been made. Notwithstanding these statements, Applicant respectfully submits that claimed invention does more than mere manipulation of data. Independent claim 5, for example, defines a method for use in deriving fixed bond information that comprises the steps:

- analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;
- identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
- evaluating at least a subset of the fixed bond representation candidates;
- selecting from among the plurality of fixed bond representation candidates based on the evaluation; and
- producing fixed bond information based on the selection.

The delocalized representation of the chemical structure is analyzed and a plurality of fixed bond representation candidates are identified. At least a subset of the candidates are evaluated, in part, to allow selection of certain candidates. Next, fixed bond information is produced based on the selection. The fixed bond information is useful, for example, to help derive chemical structure diagrams from chemical names, as set forth in the disclosure. Page5, lines 6-7.

It is therefore respectfully submitted that claims 5-20 satisfy the requirements of 35 U.S.C. §101.

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

Claims 5-21 were rejected under 35 U.S.C. §112, second paragraph as being indefinite for failing to particularly point out and distinctly claim the subject matter regarded as the invention. In support of this rejection, the Office Action principally identifies various passages of the disclosure and the claims that appear to result in confusion with regards to the terms Kekulé structure and fixed bond. The Office Action also suggests that the wording of these terms do not properly define the metes and bounds of the claims.

Applicant has reviewed and made amendments to the claims that should remedy all instances of indefiniteness.

It is therefore respectfully submitted that all of the pending claims now satisfy the requirements of 35 U.S.C. §112, second paragraph. Withdrawal of this rejection is respectfully requested.

Claims 5, 11, 15, and 20 were rejected under 35 U.S.C. §102(b) as being anticipated by Graovac et al. [JACS 95(19):6267-6273 (1973)]. The Office Action alleges that the Graovac abstract summarizes the description therein as being directed to the utilization of valence structures of hydrocarbon systems to produce a Kekulé index which corresponds to Kekulé-type valence structures. Table I of Graovac allegedly contains indices that are deemed to be fixed bond information as set forth in the pending claims. The tables in Graovac are also alleged as disclosing Kekulé index information in an order that supposedly amounts to the claimed priority queuing.

As amended, independent claim 5 defines a method for use in deriving fixed bond information that comprises the steps:

- analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;
- identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
- evaluating at least a subset of the fixed bond representation candidates;
- selecting from among the plurality of fixed bond representation candidates based on the evaluation; and
- producing fixed bond information based on the selection.

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

The delocalized representation of the chemical structure is analyzed and a plurality of fixed bond representation candidates are identified. At least a subset of the candidates are evaluated, in part, to allow selection of certain candidates. Next, fixed bond information is produced based on the selection.

Contrary to claim 5, Graovac appears to disclose a method that takes a particular fixed bond representation and computes its relative contribution (i.e., the Kekulé index) to the manifold of alternative valence bond depictions. The method of Graovac is only applicable to cyclic systems and all-carbon systems. Furthermore, Table 1 of Graovac only illustrates certain values that have been selected as input for calculating the Kekulé index. The diagrams only depict conventional fixed-bond drawings. Additionally, there is simply no priority queuing shown in Table 1 of Graovac. As applied to claim 5, there is simply no disclosure or suggestion in Graovac for the steps of:

- analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;
- identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
- evaluating at least a subset of the fixed bond representation candidates;
- selecting from among the plurality of fixed bond representation candidates based on the evaluation; and
- producing fixed bond information based on the selection.

It is therefore respectfully submitted that independent claim 5 is allowable over the art of record.

Claims 11 and 15 depend from independent claim 5 and are also believed allowable for at least the reasons set forth above with respect to claim 5. In addition, these claims each introduce novel elements that independently render them patentable over the art of record.

Independent claim 20 defines a system for use in deriving fixed bond information. The system comprises:

- an analyzer analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized representation describes a polycyclic ring system;

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
an evaluator evaluating at least a subset of the fixed bond representation candidates;
a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and
a producer producing fixed bond information based on the selection.

The components of claim 20 can provide, at least in part, functions that are similar to the steps recited in claim 5. As previously stated, Graovac does not disclose or suggest these features.

It is therefore respectfully submitted that independent claim 20 is allowable over the art of record.

Claims 5, 7, 8, 10, 11, 15, and 19-21 were rejected under 35 U.S.C. §102(b) as being anticipated by Morikawa [Computers Chem. 20:159-165 (1996)]. In support of this rejection, the Office Action indicates that Morikawa discloses the analysis of Kekulé structure representations of polycyclic chemicals with specific structures in Figures 1-3. The Office Action alleges that Morikawa analyzes, identifies, and evaluates K number with the selection of specific structures. Morikawa is also alleged as depicting the production of fixed bond information as required by claims 5, 20, and 21. The bonding shown in the figures allegedly corresponds to electronic state and valence distribution and priority queuing. Portions of the structures in Figures 2 and 3 are alleged as being non-cyclic or acyclic, while Figure 3 shows a pair of radicals. The Office Action also indicates that the structures in Figures 1-3 include a monocyclic portion.

As amended, independent claim 5 defines a method for use in deriving fixed bond information that comprises the steps:

analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;
identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
evaluating at least a subset of the fixed bond representation candidates;
selecting from among the plurality of fixed bond representation candidates based on the evaluation; and
producing fixed bond information based on the selection.

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

The delocalized representation of the chemical structure is analyzed and a plurality of fixed bond representation candidates are identified. At least a subset of the candidates are evaluated, in part, to allow selection of certain candidates. Next, fixed bond information is produced based on the selection.

Applicant has reviewed Morikawa and respectfully disagrees with the interpretation thereof by the Office Action. Morikawa appears to produce fixed-bond representations of PBHCs from a mathematical formula. There does not appear to be any disclosure of how such fixed bond representations could be produced from a delocalized drawing or representation. Morikawa appears to be limited to certain types of all-carbon systems. Furthermore, the figures in Morikawa do not illustrate the electronic state and valence distribution of the structures, as asserted in the Office Action. Importantly, there is simply no disclosure or suggestion in Morikawa for the steps recited in independent claim 5 such as:

- analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized structure representation describes a polycyclic ring system;
- identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
- evaluating at least a subset of the fixed bond representation candidates;
- selecting from among the plurality of fixed bond representation candidates based on the evaluation; and
- producing fixed bond information based on the selection.

It is therefore respectfully submitted that independent claim 5 is allowable over the art of record.

Claims 7, 8, 11, 15, and 19 depend from independent claim 5, and are therefore believed allowable for at least the reasons set forth with respect to claim 5. In addition, these claims each introduce novel elements that independently render them patentable over the art of record.

Independent claims 10 defines a method for use in deriving fixed bond information that comprises, in part, the steps:

- ... identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

evaluating at least a subset of the fixed bond representation candidates;
selecting from among the plurality of fixed bond representation candidates based on the evaluation;
producing fixed bond information based on the selection ...

As previously discussed with respect to independent claim 5, these steps are neither taught nor suggested by Morikawa.

It is therefore respectfully submitted that independent claim 10 is allowable over the art of record.

Independent claim 20 defines a system for use in deriving fixed bond information. The system comprises:

- an analyzer analyzing a delocalized representation of a chemical structure, wherein at least a portion of the delocalized representation describes a polycyclic ring system;
- an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
- an evaluator evaluating at least a subset of the fixed bond representation candidates;
- a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and
- a producer producing fixed bond information based on the selection.

The components of claim 20 can provide, at least in part, functions that are similar to the steps recited in claim 5. As previously stated, Morikawa simply fails to either disclose or suggest these features.

It is therefore respectfully submitted that independent claim 20 is allowable over the art of record.

Independent claim 21 defines computer software, residing on a computer-readable medium that comprises a set of instructions. The instructions cause a computer system to:

- analyze a delocalized representation of a chemical structure, wherein at least a portion of the delocalized representation describes a polycyclic ring system;
- identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
- evaluate at least a subset of the fixed bond representation candidates;

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

select from among the plurality of fixed bond representation candidates based on the evaluation; and
produce fixed bond information based on the selection.

The steps performed by the computer system of claim 21 are somewhat similar to the steps performed in independent claim 5. As previously discussed, Morikawa fails to disclose or in any way suggest such features.

It is therefore respectfully submitted that independent claim 21 is allowable over the art of record.

For the reasons stated above, it is respectfully submitted that all of the pending claims (5-16 and 19-21) are now in condition for allowance. Therefore, a Notice of Allowance is believed in order, and courteously solicited.

The Examiner is respectfully requested to contact the undersigned, if it is believed that such contact would further the examination of the present application.

Application Serial No. 09/506,717
Amendment dated April 23, 2004
Reply to Office Action dated October 23, 2003

AUTHORIZATION

The Commissioner is hereby authorized to charge any additional fees that may be required for this Response, or credit any overpayment, to deposit account number 08-0219.

In the event that an extension of time is required, or which may be required in addition to that requested in a petition for an extension of time, the Commissioner is requested to grant a petition for that extension of which is required to make this response timely, and is hereby authorized to charge any fee for such, to deposit account number 08-0219.

Respectfully submitted,



Leonid D. Thenor

Reg. No. 39,397

Hale and Dorr LLP
Willard Office Building
1455 Pennsylvania Ave., N.W.
Washington, DC 20004
202-942-8400
April 23, 2004